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Title: ROBUSTNESS-TO-UNCERTAINTY, FIDELITY AND PREDICTION-LOOSENESS OF MODELS (U)

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Los Alamos
NATIONAL LABORATORY

ROBUSTNESS-TO-UNCERTAINTY, FIDELITY-TO-DATA, PREDICTION-LOOSENESS OF MODELS (U)

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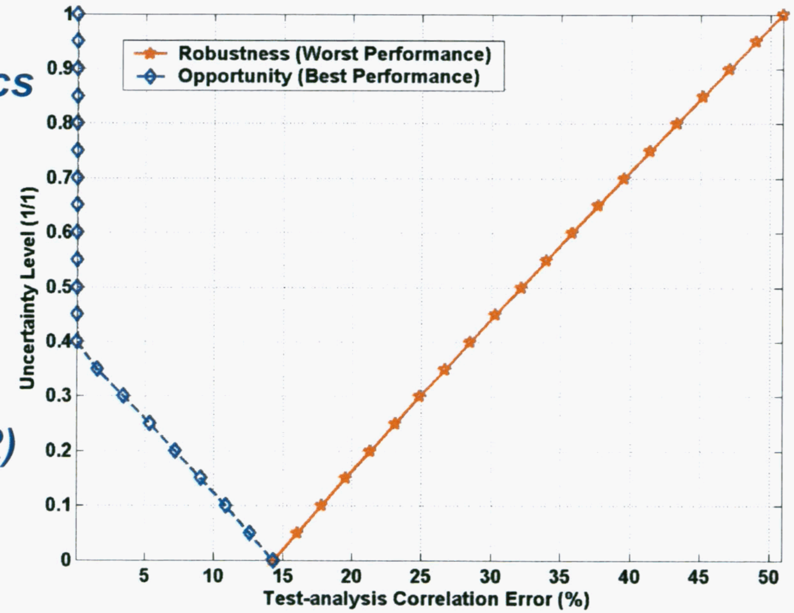

Abstract

A key aspect of science-based predictive modeling is to assess the credibility of predictions. To gain confidence in predictions, one should demonstrate consistency between physical observations, expert judgments, and the predictions of equally credible models. This suggests a relationship between fidelity-to-data, robustness-to-uncertainty, and confidence in prediction. The purpose of this work is to explore the interaction between these three aspects of predictive modeling. The concepts of fidelity, robustness, and confidence are first defined in a broad sense. A Theorem is then proven that establishes that these three objectives are antagonistic. This means that high-fidelity models cannot, at the same time, be made robust to uncertainty and lack-of-knowledge. Similarly, equally robust models cannot provide consistent predictions, hence reducing confidence. The conclusion of this theoretical investigation is that, in assessing the predictive accuracy of numerical models, one should never focus on a single aspect only. Instead, the trade-offs between fidelity-to-data, robustness-to-uncertainty, and confidence in prediction should be explored.

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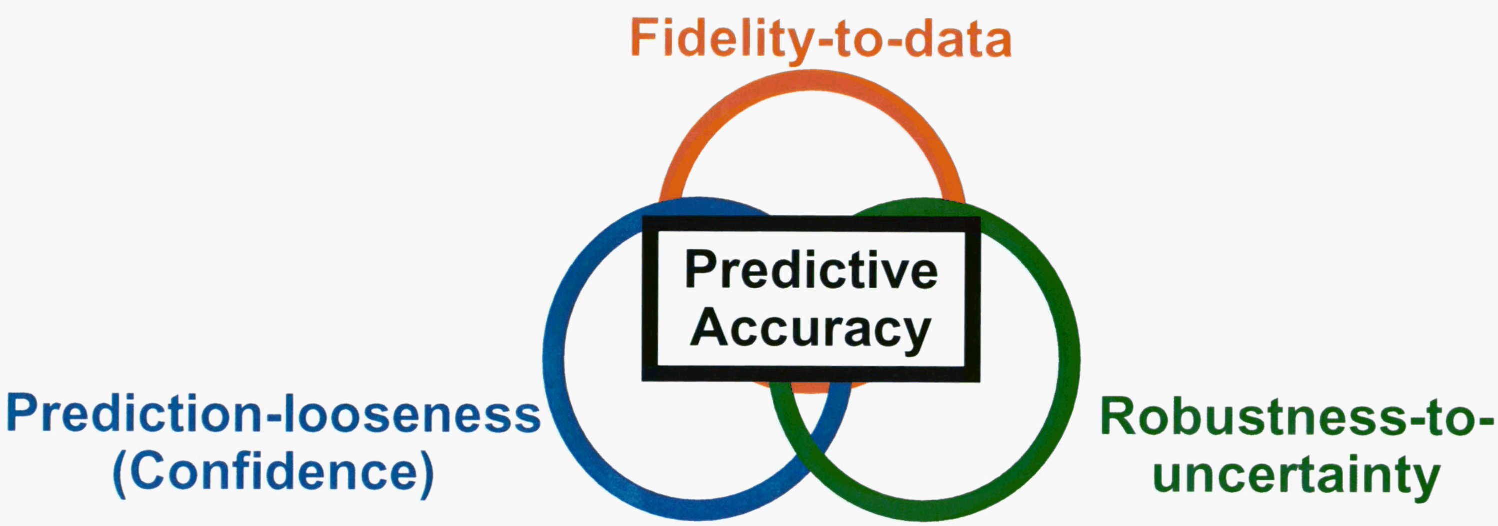
Purpose

- Explore the relationship between three aspects of science-based predictive modeling:



- Our thesis is that prediction *credibility* cannot be achieved without first understanding the trade-offs between fidelity, robustness, and confidence.

The Relationship Between Experiments and Simulations is Changing …

- *Old paradigm:*

  Experiments are qualification tests, proof that something does or does not “break”. Simulations are used to understand what happened, generally, after the fact.

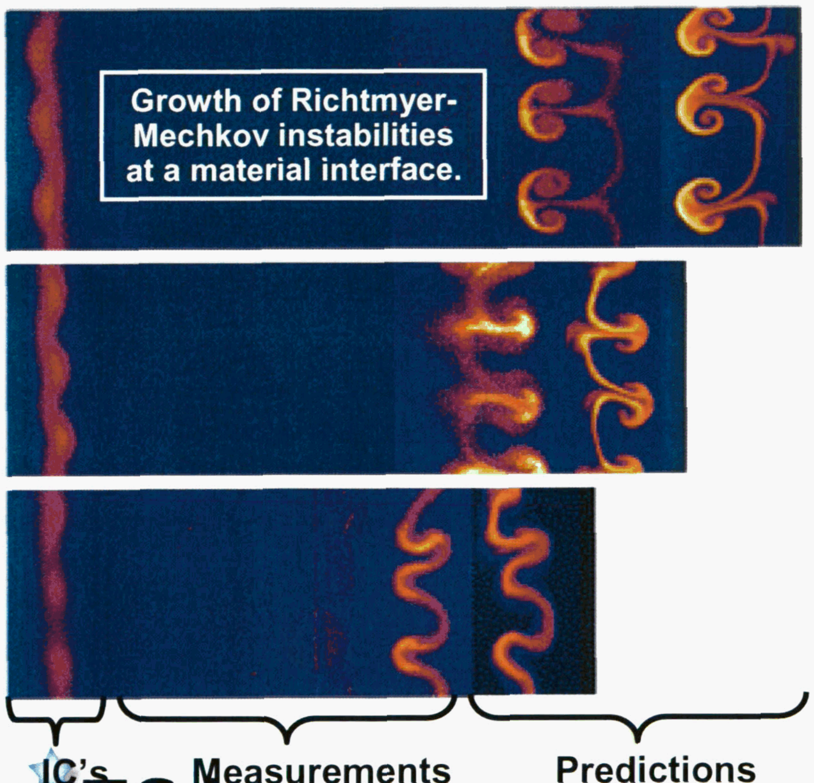
- *New paradigm:*

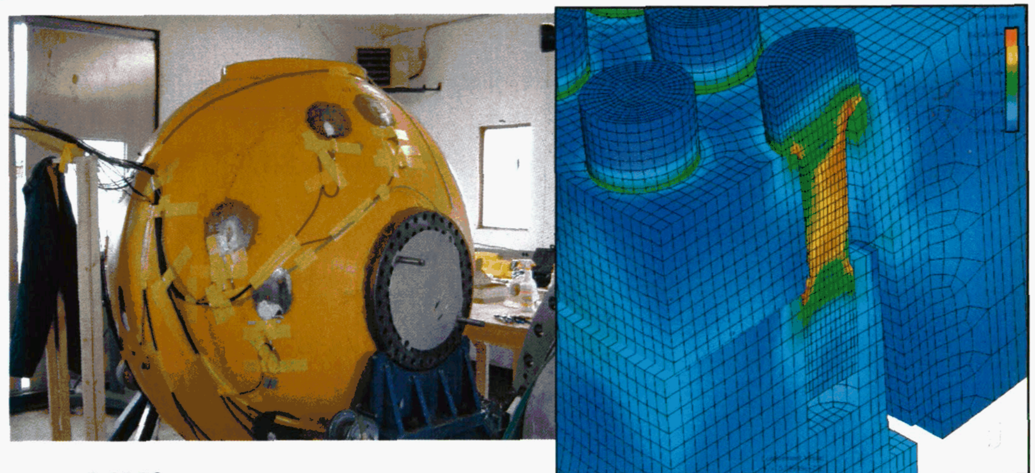
  Experiments explore the mechanics and validate predictions. Simulations are used to predict, with *quantifiable confidence* , across the *operational space*.

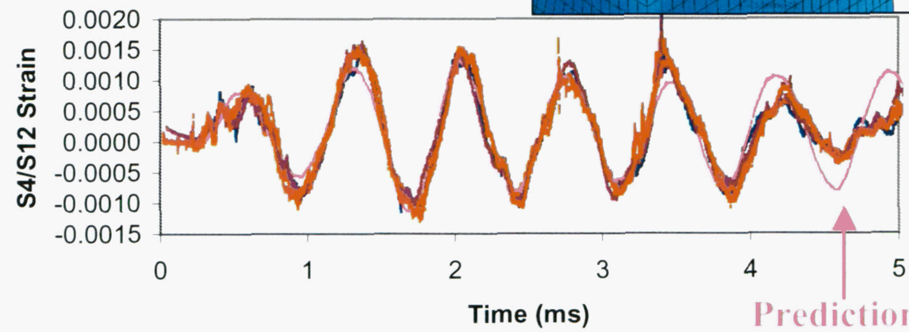
➡ *Key:* Demonstrate the *credibility* of predictions.

M&S Examples

- **Predictability can be achieved if the right physics, loading, and initial conditions are included in the computational model.**







Simulation of a Potential Leak Path in Containment Vessels

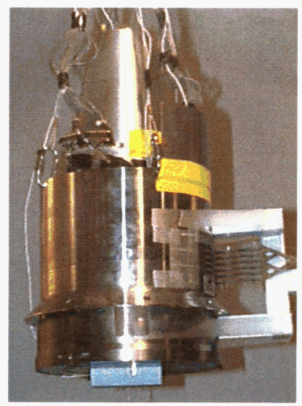
Information Integration

- Modeling & Simulation (M&S) is not sufficient to achieve credible predictability. Information from other sources must be integrated.

First-physics Principles

$$\boxed{F = m\frac{\partial^2}{\partial t^2}X(t)}$$

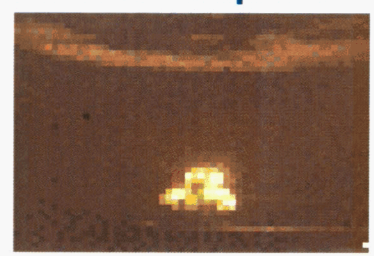
Test & Experimental Observables



Expert Judgment

Modeling & Simulation

Historical Experience

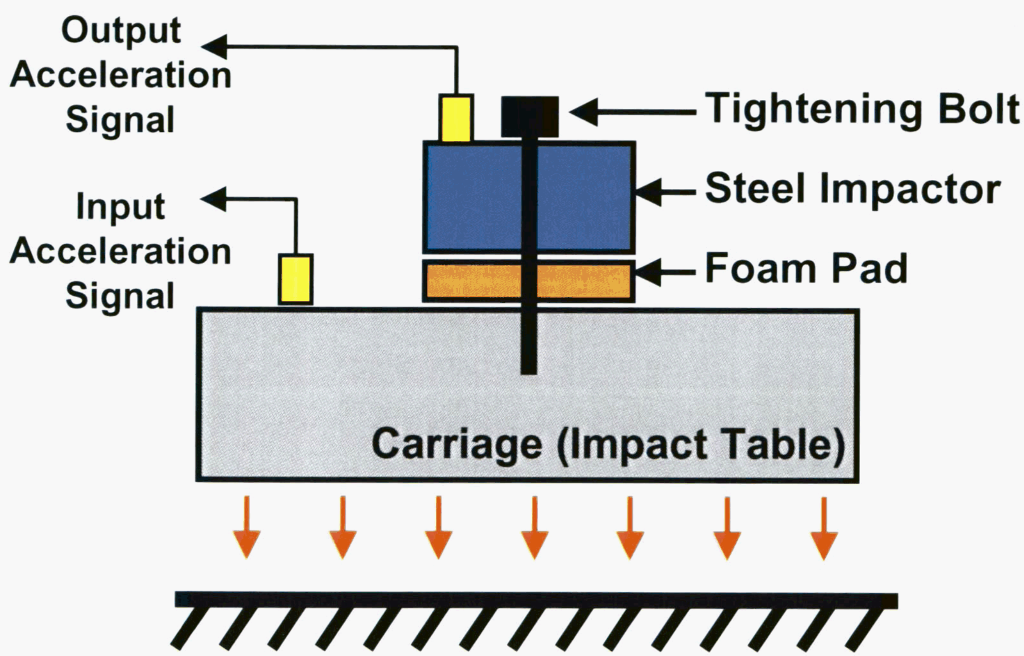


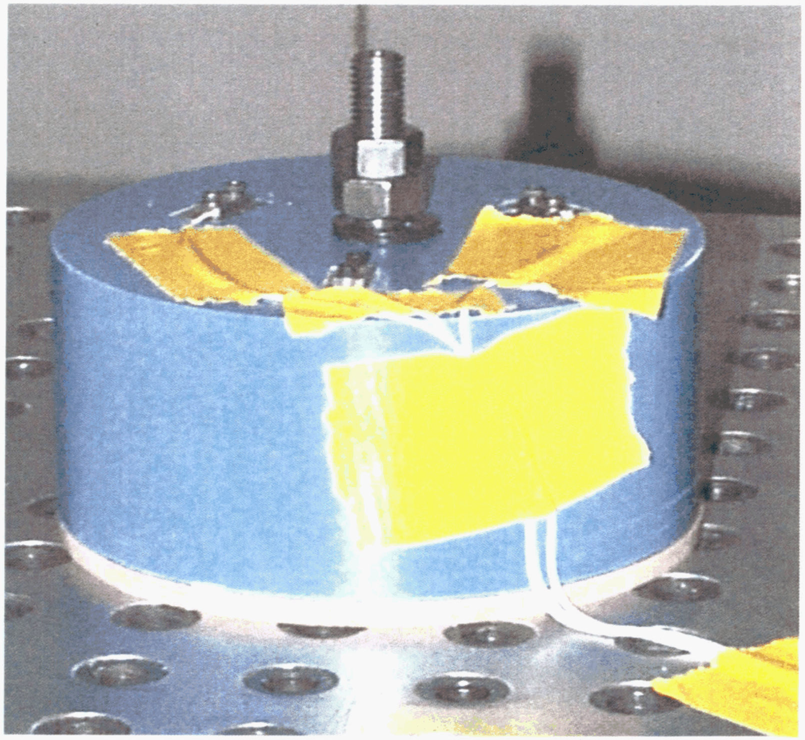
Knowledge & Intuition

→ *Goal:* Combine *all* we know and determine *how well* we know it.

Engineering Application

- The engineering application is the propagation of an impact through an assembly of metallic and crushable (foam pad) components.

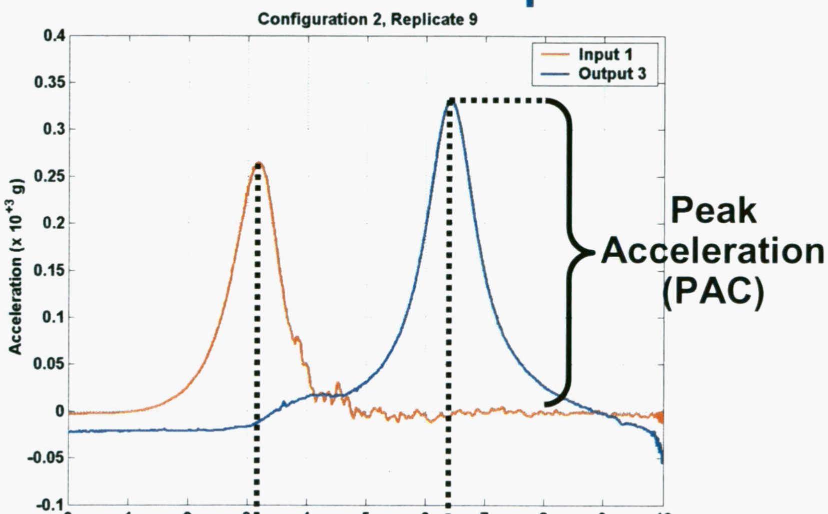


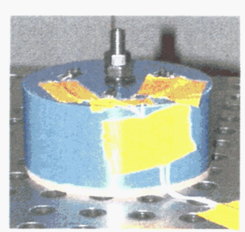


The Design Space

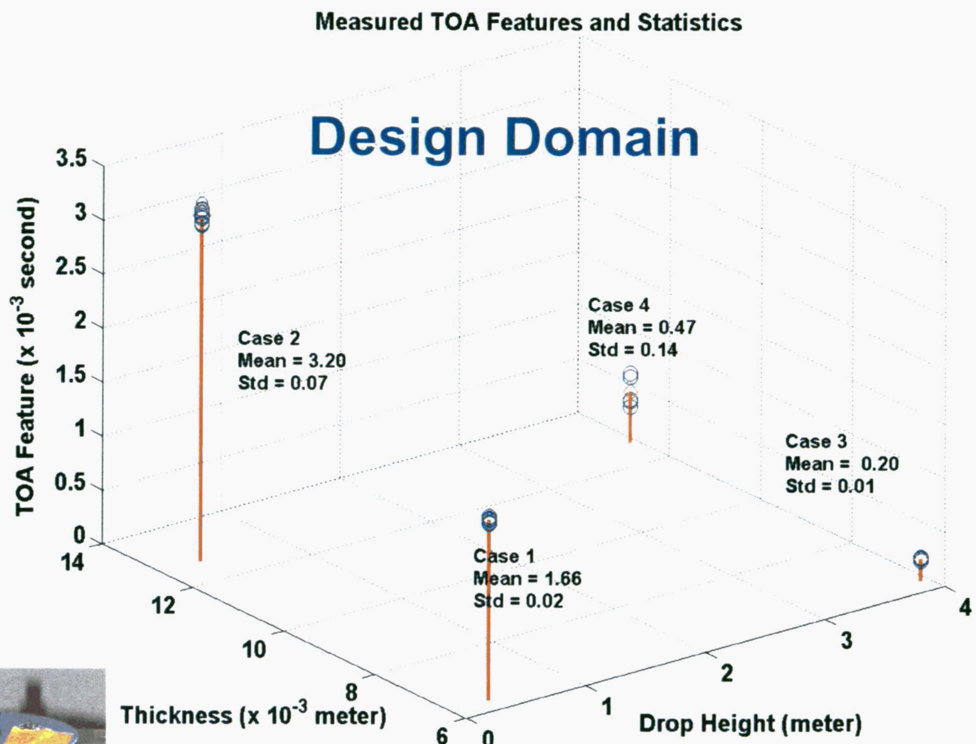
- Predictions are required for various combinations of foam pad thickness and impact load magnitude.

Features of the Response



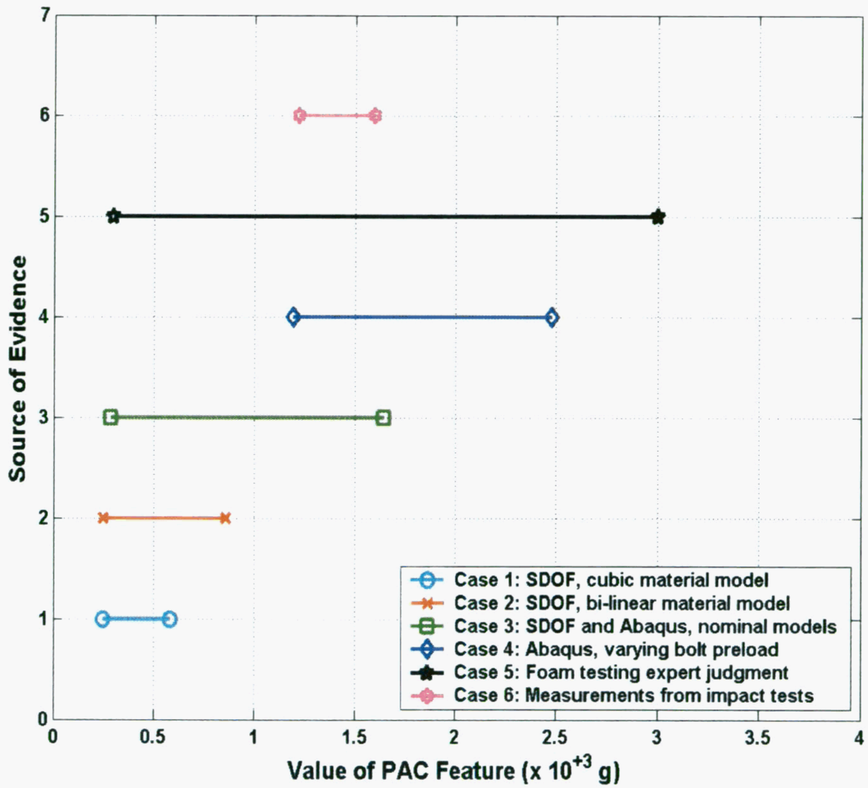


Design Domain



Sources of Evidence

- Evidence about the value of the peak acceleration (PAC) feature come from several sources.



Test measurements

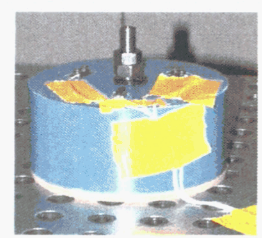
Expert judgment

Simulations from high-fidelity finite element models

Simulations from low-fidelity finite element models

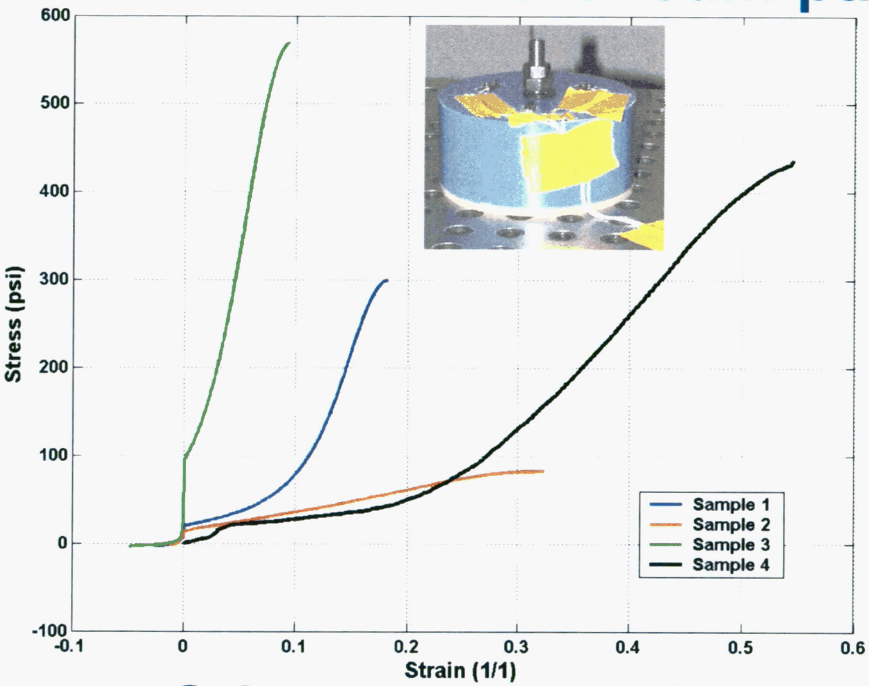
Simulations from SDOF models

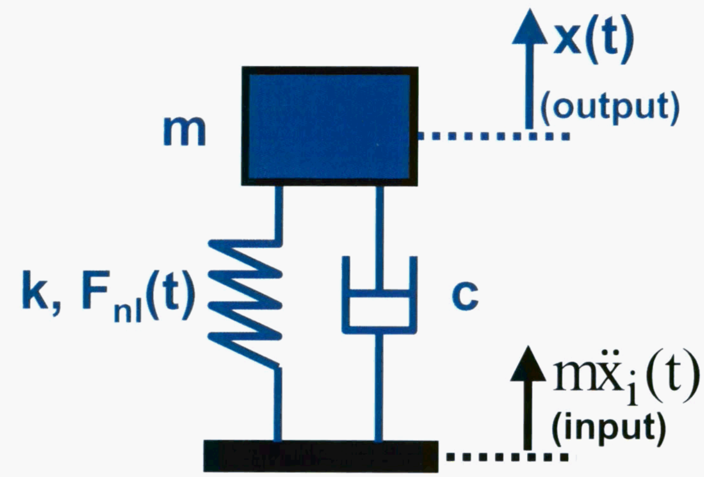
Simulations from SDOF models



Material Uncertainty

- The main modeling uncertainty is the constitutive material of the foam pad (strain-stress curve).





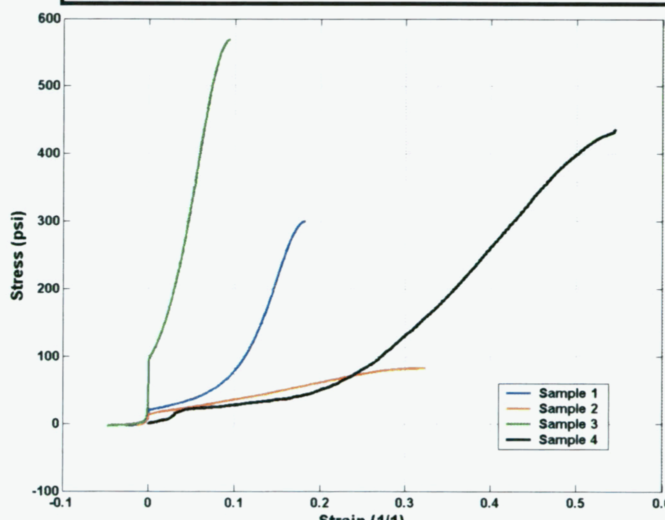
$$m\ddot{x}(t)+c\dot{x}(t)+kx(t)+F_{nl}(t)=m\ddot{x}_i(t)$$

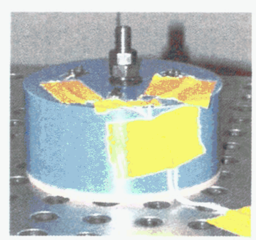
- Other sources of uncertainty include the values of the *(m;c;k)* parameters, the initial condition, and the shape and magnitude of the input acceleration.

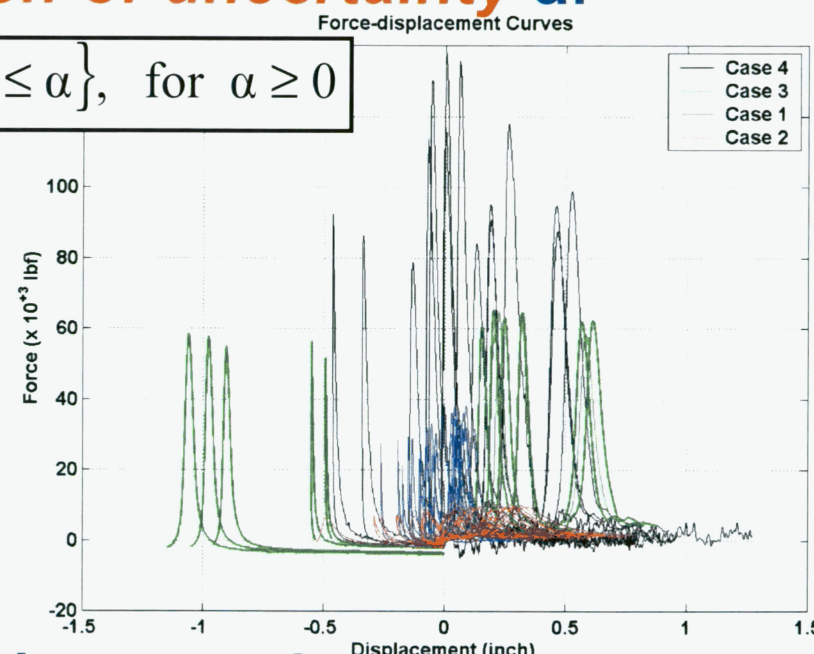
Convex Models of Uncertainty

- The uncertainty is represented by defining a family of nested, convex domains *U(α;q_o)* that "envelope" the data for a given *horizon-of-uncertainty α*.

$$U(\alpha;q_o)=\{y=M(p;q) \text{ such that } \|q-q_o\|\le\alpha\}, \quad \text{for } \alpha\ge 0$$







- At any horizon-of-uncertainty, strain-strain curves can be "realized" from a domain *U(α;q_o)*, and used to define the non-linear forcing function $F_{nl}(t)$.

Typical Difficulties

- Experimental data sets are sparse and uncertain. Expert judgment is often ambiguous. Models have distributions on their outputs.

- Modeling assumptions provide a false sense of confidence by "hiding" the *lack-of-knowledge*.

- More often than not, no evidence is available to suggest that these sources of uncertainty follow conventional probability distributions.

- Similarly, no evidence is often available to suggest degrees of belief, membership functions, basic probability assignments, or possibility structures.

Path Forward

- To demonstrate credibility (or provide confidence), the sources of uncertainty and their influence on the predictions must be assessed.
- This work does not advocate alternate approaches to probability theory to represent the uncertainty.
- Nevertheless, each source of uncertainty should be represented using the most appropriate theory. (The difficulty becomes information integration.)
- The two important questions are:
  - ➡ *What is the total uncertainty?*
  - ➡ *Are decisions robust to the uncertainty?*

Definitions

- ***Fidelity-to-data (R)*: Degree of correlation between test data and simulation predictions.**

$$R^2 = \sum_{k=1\ldots N_{Test}} \left(y_{Test}^{(k)} - M(p^{(k)};q) \right)^2$$

- ***Robustness-to-uncertainty (α*)*: Maximum value of the horizon-of-uncertainty for which all models of the corresponding family *U(α;q$_o$)* meet a given fidelity requirement *R$_{Max}$*.**

$$\alpha^* = \max_{\alpha \geq 0} \left\{ R \leq R_{Max}, \text{ for all } M \in U(\alpha;q_o) \right\}$$

- ***Prediction-looseness (λ$_Y$)*: Range of predictions expected from a family of equally-credible models.**

$$\lambda_Y = \max_{M \in U(\alpha^*;q_o)} M(p;q) - \min_{M \in U(\alpha^*;q_o)} M(p;q)$$

Two Important Remarks …

- The importance of "prediction-looseness" stems from the fact that, to predict with confidence, there should be little difference (or small looseness λ_Y) between predictions of equally-credible models.

- Assessing the confidence in prediction here refers to an assessment of prediction error away from settings where physical experiments have been performed.

Theorem

- *Theorem:* Let $U(\alpha;q_o)$ be an info-gap family of models that obeys the axioms of nesting and translation. Let α^* be its robustness function. Consider two initial settings of model parameters, q_o and q_o'. If $\alpha^*(q_o) \geq \alpha(q_o')$, then $\lambda_Y(q_o) \geq \lambda_Y(q_o')$.

$$\boxed{\text{Theorem}: \quad \frac{\partial \alpha^*}{\partial R} \geq 0, \quad \frac{\partial \lambda_Y}{\partial \alpha^*} \geq 0, \quad \frac{\partial \lambda_Y}{\partial R} \geq 0}$$

- Fidelity-to-data *R* and robustness-to-uncertainty α^* are *antagonistic*.

- Robustness-to-uncertainty α^* and looseness λ_Y (or confidence-in-prediction) are *antagonistic*.

Trade-offs Established by the Theorem

- *Robustness decreases as fidelity improves.*

  Numerical simulations calibrated to better reproduce the available test data become more vulnerable to errors in modeling assumptions, errors in the functional form of the model, and uncertainty and variability in the model parameters.

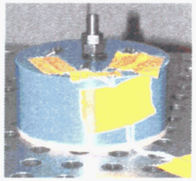
- *Looseness increases as robustness improves.*

  Numerical simulations that are made more immune to uncertainty and modeling errors provide a wider, hence less consistent, range of predictions.

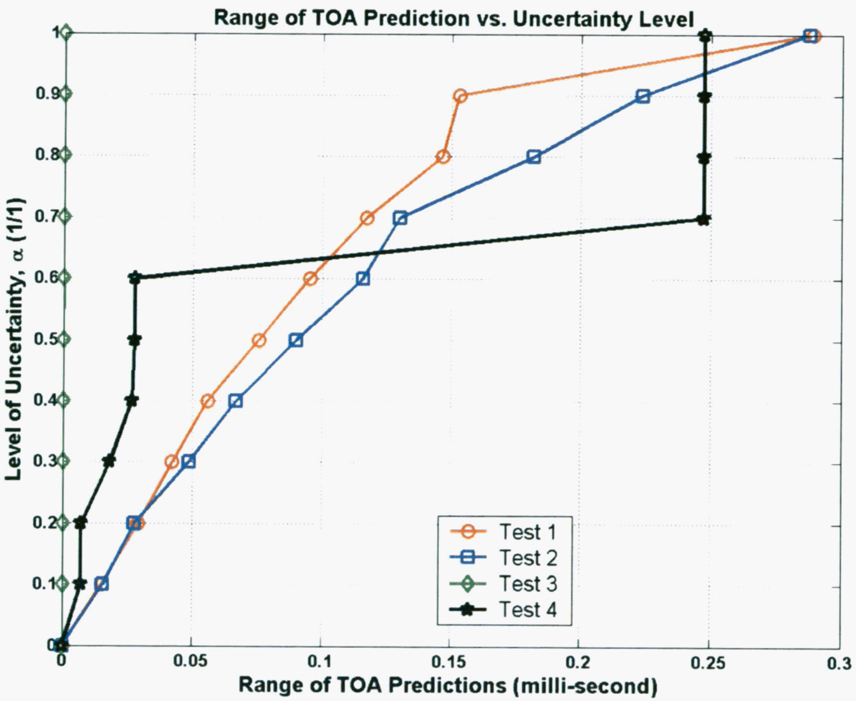
- *Looseness decreases as fidelity improves.*

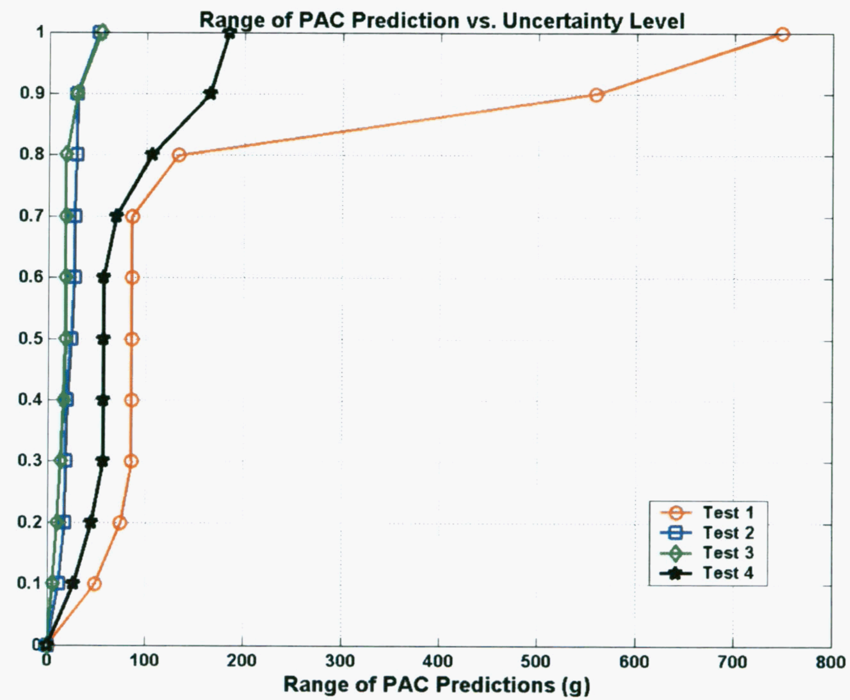
  Numerical simulations made to better reproduce the available test data provide more consistent predictions. May lead to "over-calibrating" and a false sense of confidence.

Results — 1

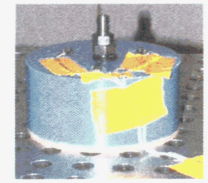


- Ranges of TOA and PAC predictions for increasing α-levels of uncertainty.

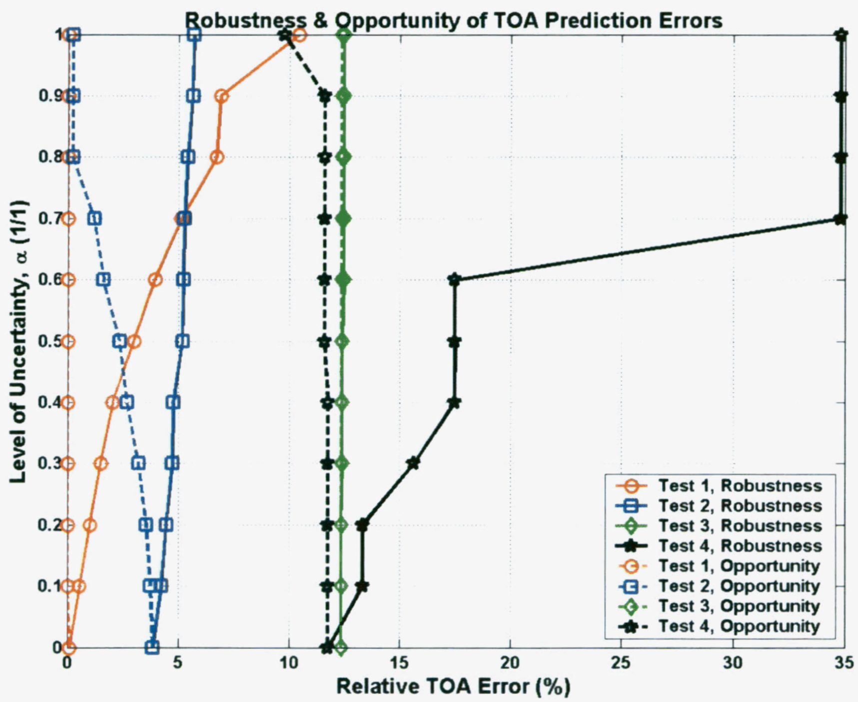


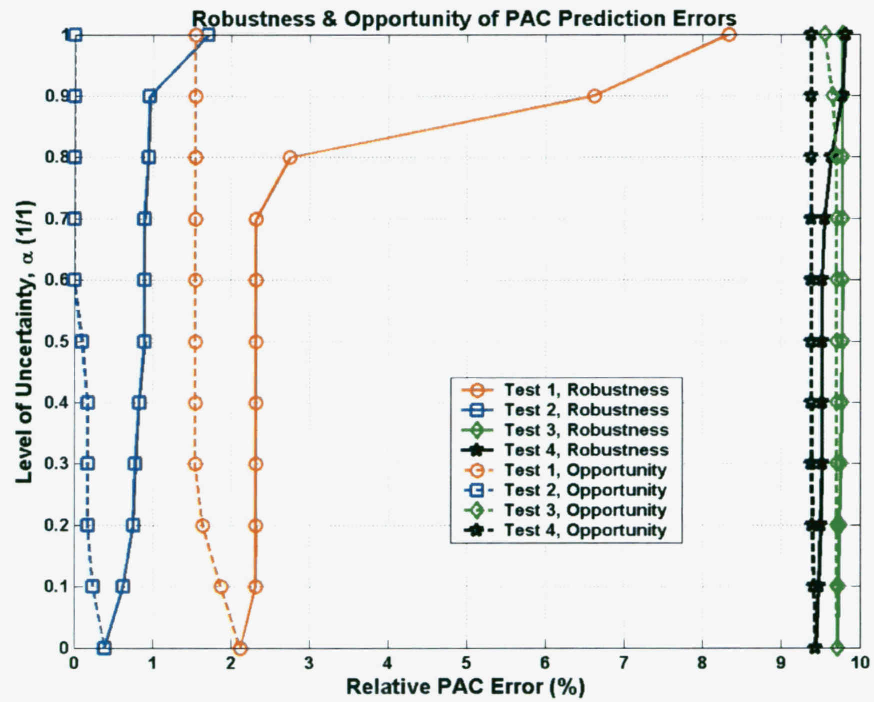


Results — 2

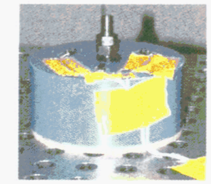


- Robustness and opportunity of prediction errors for increasing α-levels of uncertainty.

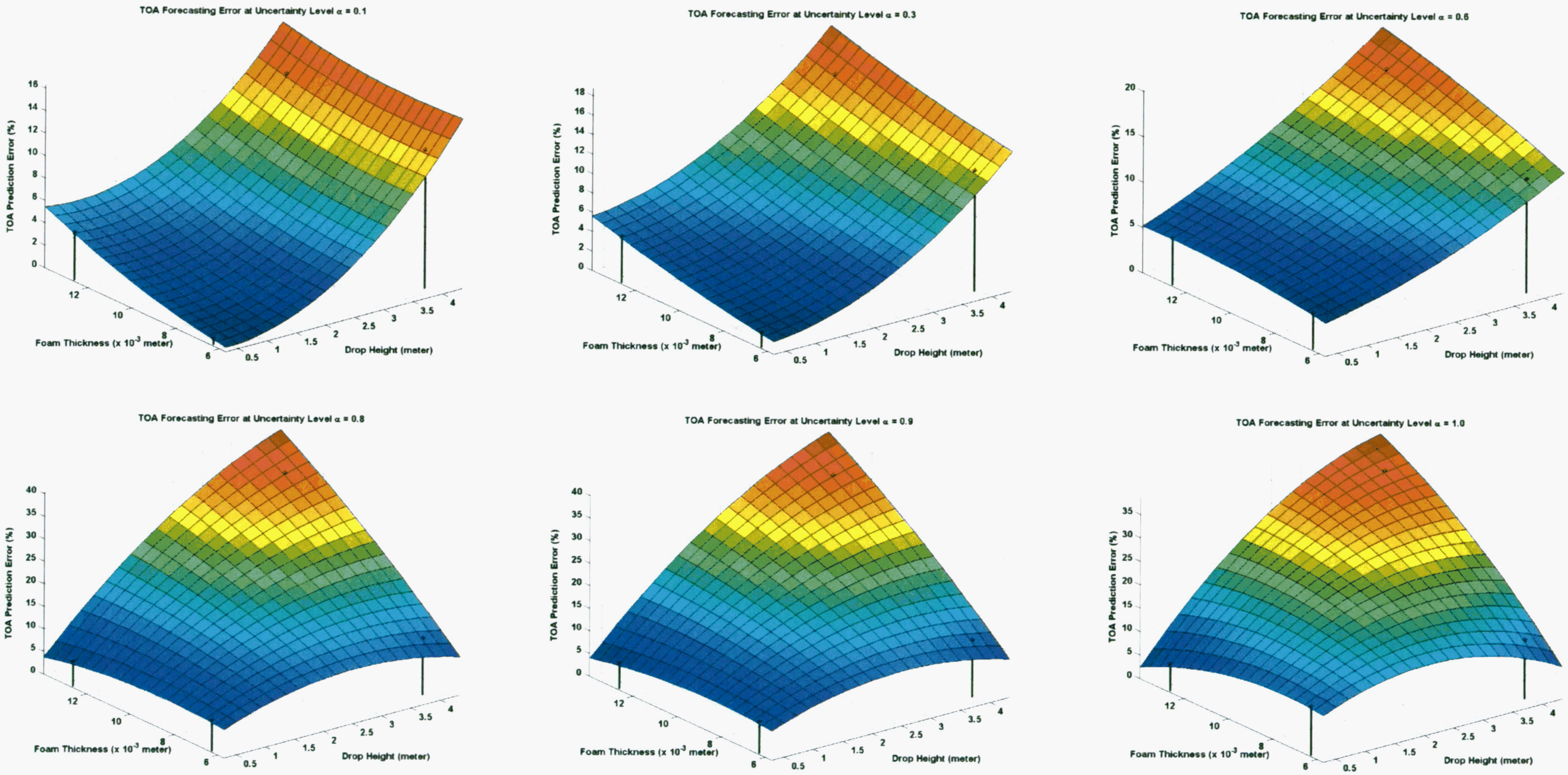




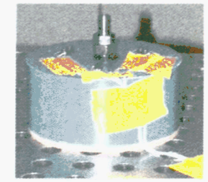
Results — 3



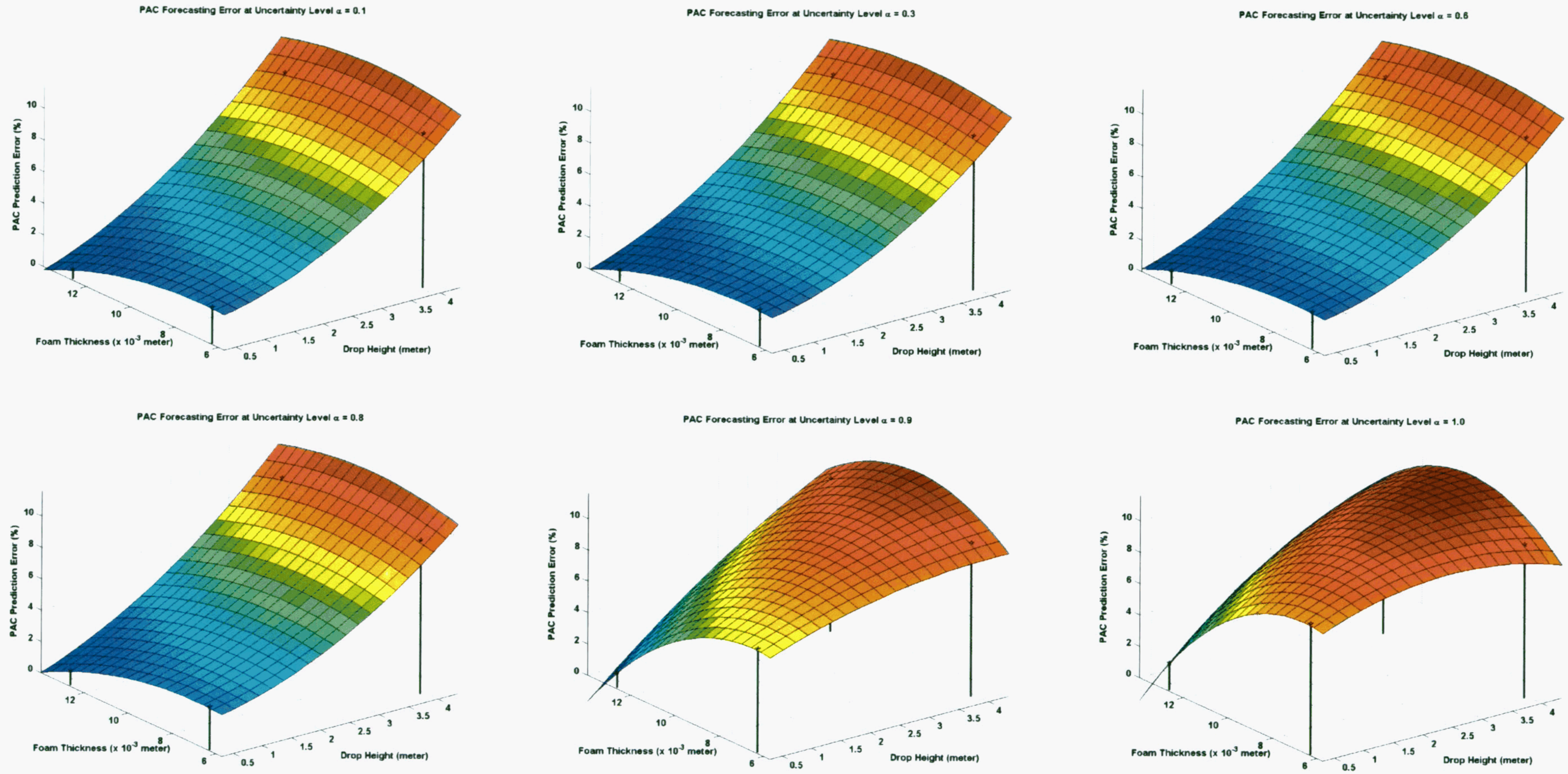
- TOA forecasting errors for several α-levels.



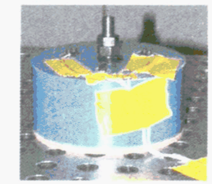
Results — 4



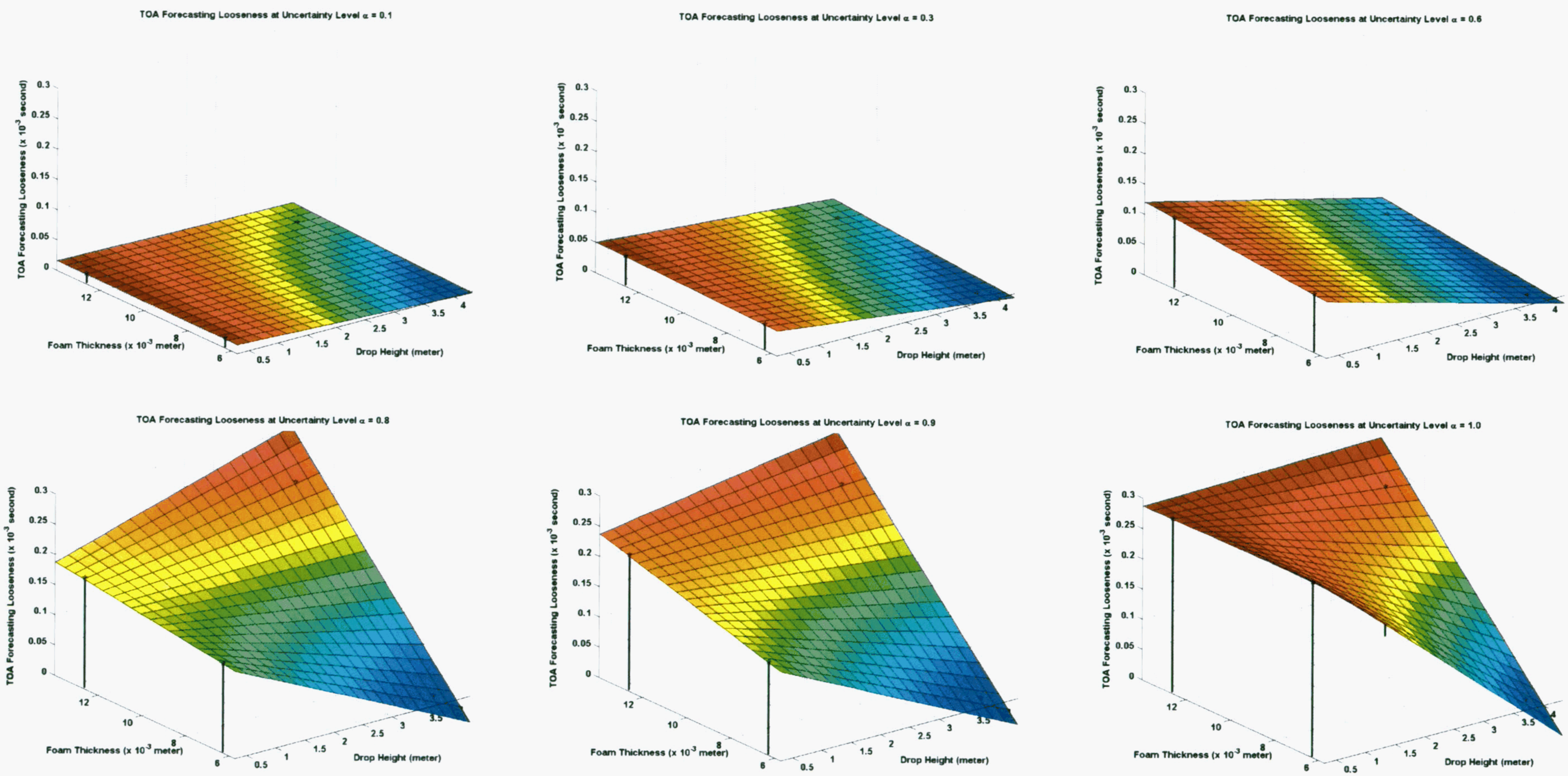
- PAC forecasting errors for several α-levels.



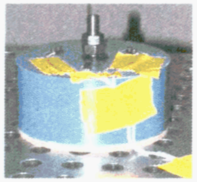
Results — 5



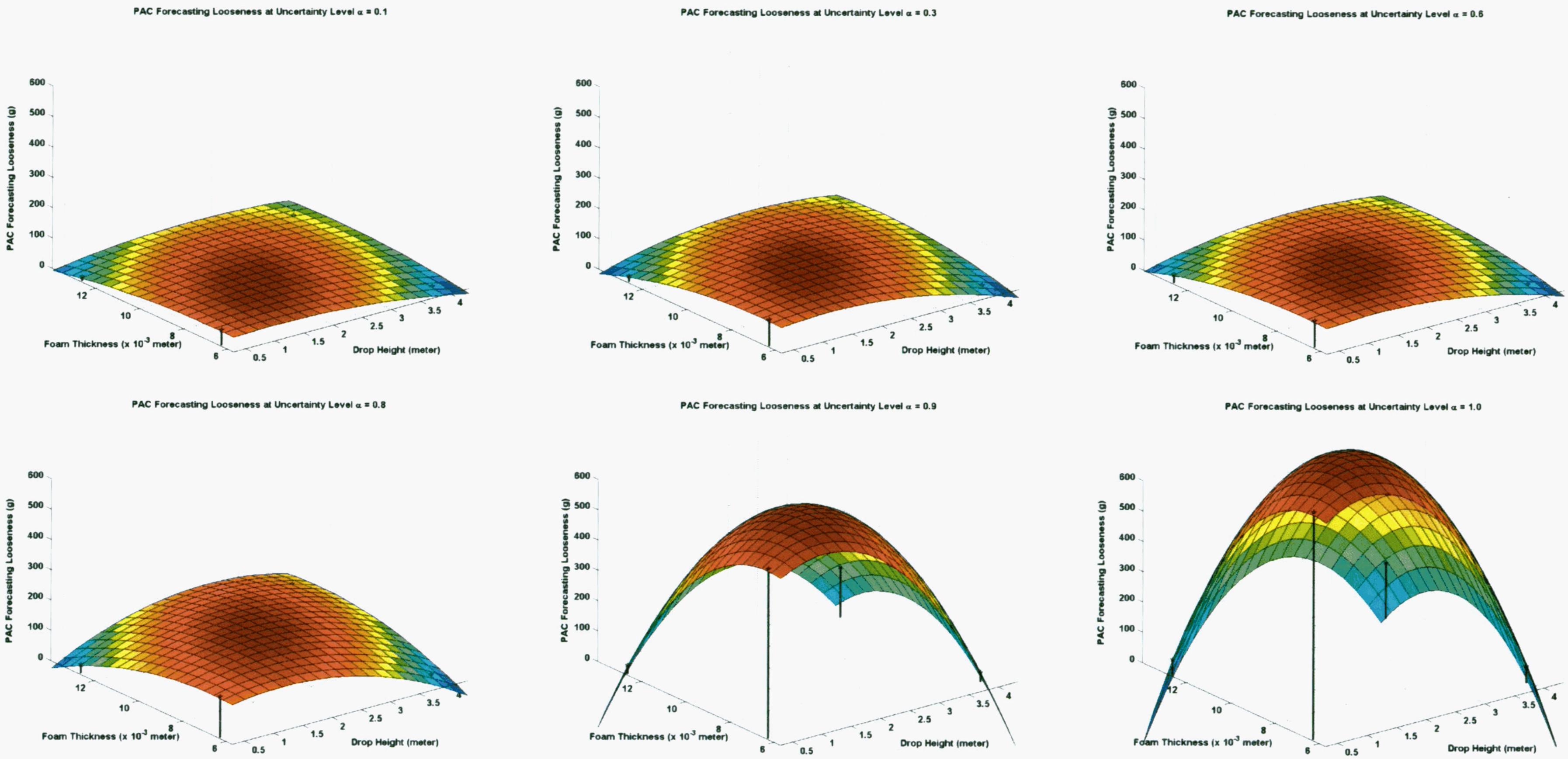
- TOA looseness (range) for several α-levels.



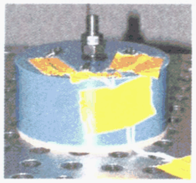
Results — 6



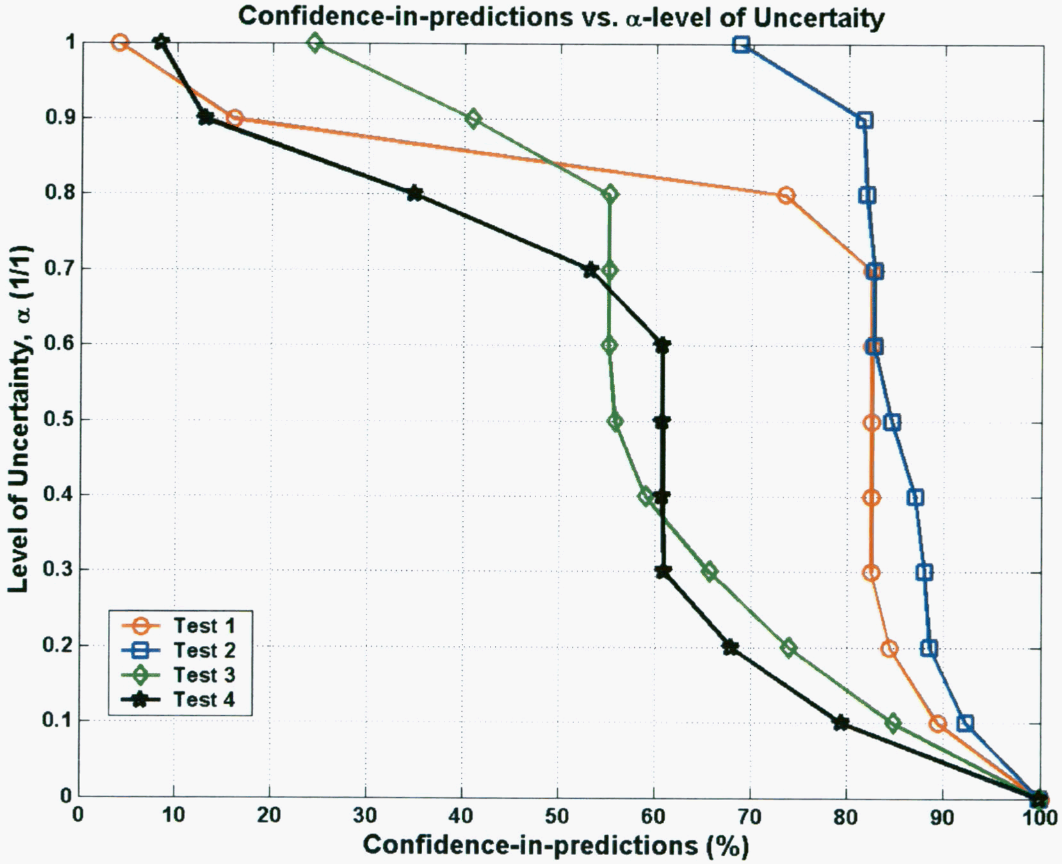
- PAC looseness (range) for several α-levels.



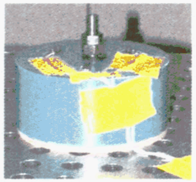
Results — 7



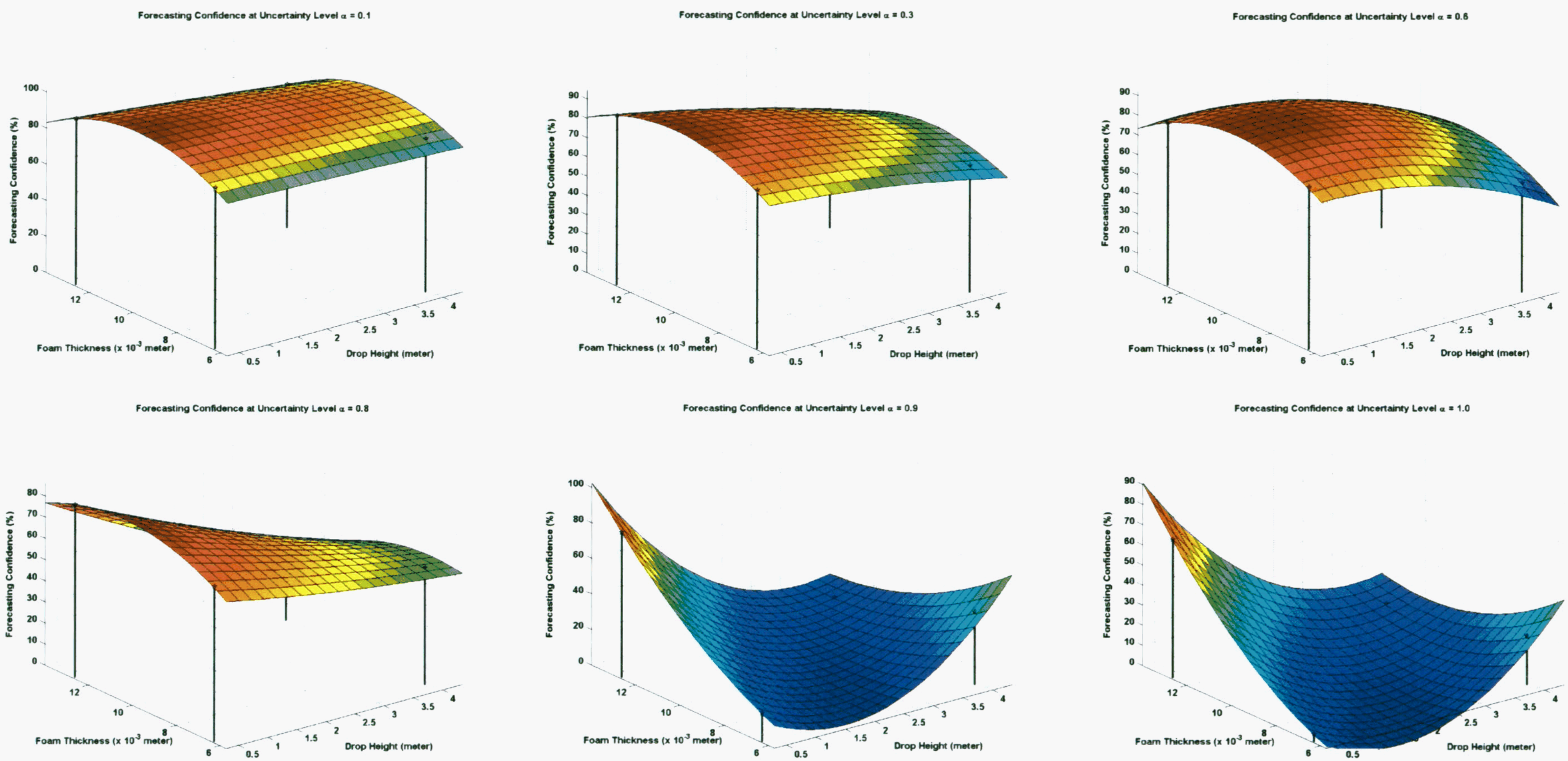
- Confidence-in-predictions (derived from TOA and PAC "looseness" using the total uncertainty, *TU*).



Results — 8



- Confidence-in-prediction for several α-levels.



Conclusion

- Prediction *credibility* cannot be achieved without understanding the trade-offs between fidelity, robustness, and confidence.
- Calibrating numerical simulations for maximum fidelity-to-data is *not* a sound decision-making strategy.
- Fidelity-to-data does *not* imply model validation. In fact, optimized models have *zero* robustness to uncertainty.
- Instead of being optimized, fidelity-to-data should be made "good enough." Robustness-to-uncertainty and / or confidence-in-prediction should be optimized, but remember that the two are antagonistic.